coupling effects on the level of perturbation theory, demonstrate that magnetic moments of molybdenum atom should be oriented along easy axis, which corresponds to anisotropic energy minimum. Utilisation of INS revealed the clear magnetic excitations at 20 meV, and fitting of them also gives the easy axis, where anisotropic terms are in reasonable agreement with theory (Fig.1).

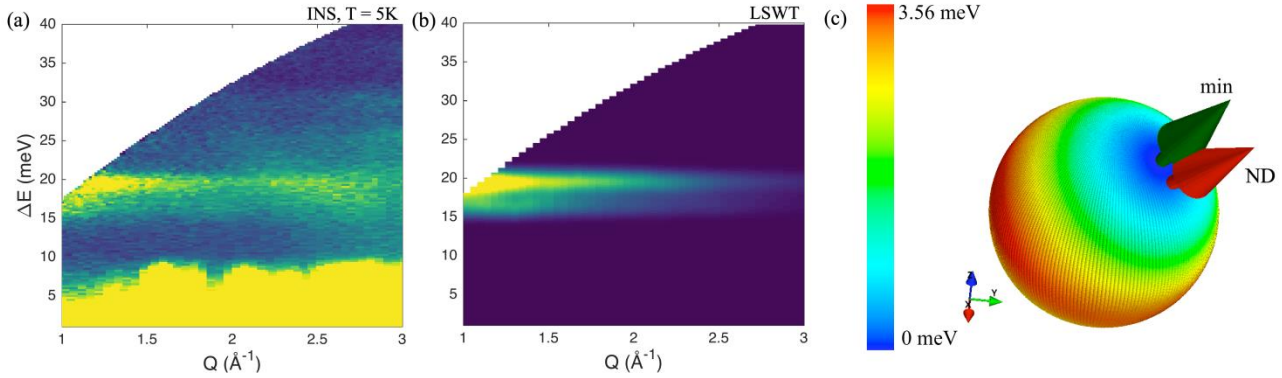

Fig. 1. (a) Inelastic neutron scattering spectra obtained for powder sample of $BaMoP_2O_8$.(b) The fitted spectra by using anisotropic spin model. (c) The 3D map of anisotropic energy, obtained on the level of DFT+U method. The green arrow denoted as «min» corresponds to minimum of anisotropic energy, while the red arrow «ND» — easy axis from neutron experiment.

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STRUCTURE OF CDTE NANOCRYSTALS SYNTHESIZED BY ELECTROCHEMICAL DEPOSITION FROM DIFFERENT SOLUTIONS ONTO THE SIO_2/SI TRACK TEMPLATE

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The main aim of this study is CdTe nanocrystals growing by electrochemical deposition in the a-SiO_2/Si -n track template.

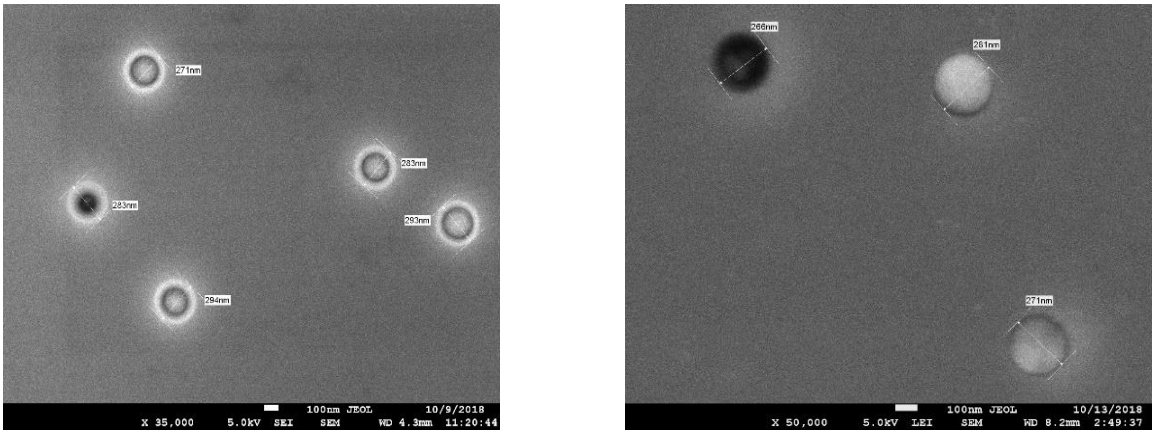
CdTe is a direct bandgap semiconductor group $A^{II}B^{VI}$ with E_g=1.49 eV at 300 K [1]. It is known that CdTe is one of the materials most suitable for solar cells production [2]. Nanocrystals, such as CdSe, ZnS, ZnSe, CdS and PbS, have nonlinear optical susceptibility, which makes it possible to use them as materials for passive optical shutters for the generation of ultrashort laser pulses in the near-IR range [3, 4].

The a-SiO_2/Si-n structure was created by thermally wet oxidizing silicon substrates in oxygen atmosphere at a temperature of 900°C. The thickness of the obtained silicon dioxide layer was 600 nm. To obtain track templates, the a-SiO2/Si-n structures were irradiated by Xe ions with 200 MeV and fluence 108 ion/cm^2 at a DC-60 accelerator (Astana, Kazakhstan). Subsequent chemical etching in an aqueous solution of hydrofluoric acid leads to the formation of nanopores. For electrochemical deposition of CdTe we used two types of solutions:

1) 1M $CdSO_4$ + 1mMTeO_2. $CdSO_4$ dissolved in water, TeO_2 –in the minimum amount of concentrated sulfuric acid. pH = 2;

2) 1M $CdCl_2$ + 1mMTeO_2. $CdCl_2$ dissolved in water, TeO_2 –in the minimum amount of concentrated sulfuric acid. pH = 2.

The samples surface was examined before and after deposition of CdTe using a JSM 7500F scanning electron microscope (SEM).



a b

Fig.1. SEM images of sample surfaces after CdTe deposition.
a) sulphate solution, U = 1,5 V during 10 min,b) chloride solution U= 1,5 V during 5 min

Figure 1 shows the SEM images of the surface after deposition for two types of solutions.

X-ray diffraction analysis (XRD) showed the formation of CdTe nanocrystals with the hexagonal structure and the space group P63mc (186).

The unit cell parameters for CdTe from sulfate electrolyte: a = 4.51185Å, c = 7.40234 Å; for the chloride solution, a = 4.53445 Å, c = 7.43525 Å. As can be seen, the cell parameters of CdTe grown in the chloride solution have somewhat greater values that in the sulphate solution one. Annealing in air at a temperature of 100°C within one hour leads to a decrease in the unit cell parameters (a = 4.51015 Å, c = 7.40214 Å) for a sulfate electrolyte and (a= 4.52033 Å, c = 7.42212 Å) for chloride electrolyte. A decrease in the size of CdTe nanocrystallites is observed from 11.19 nm to 10.15 nm for a sulfate electrolyte, and opposite, for chloride electrolyte an increase in the size of nanocrystallites from 11.24 nm to 18.24 nm was obtained. For both electrolytes, annealing led to an increase the degree of crystallinity of from 45.1% to 51.2% for

nanocrystals obtained from sulfate, while for chloride solutions the effect is more significant - from 54.5% to 72.6%.

As can be seen from obtained results, the use of chloride and sulphate electrolyte leads to the formation of CdTe nanocrystals with a hexagonal structure.

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TUNABLE DIMER SYSTEMS OF COBALT ATOMS ON PHOSPHORENE

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In this work we report on a comprehensive study of a dimer system, two cobalt atoms on phosphorene surface. Since each cobalt atom can be stabilized in high- and low-spin states, the couplings in this dimer system can be tuned. More specifically, it was shown that applying a small bias voltage one can change interaction between two atoms within dimer from ferromagnetic to antiferromagnetic and vice versa.

The structures containing few magnetic atoms on nonmagnetic surface is considered to be the prospective system, giving the possibility to realise the data storage and spintronic devices [1]. Recently, experimentally by using scanning tunnelling microscopy (STM) technique it was revealed that cobalt atom on black phosphorus demonstrates two novel — high (H) and low (L) spin states [2]. Low spin state has magnetisation 1 μ_B, whereas high spin state can be magnetised until ~ 2.5 μ_B. Within STM techniques it is possible to change spin states of the corresponding cobalt atom from low to high spin states and vice versa applying a small bias voltage between tip and surface. As for considering cluster of atoms, the realisation of tunable spin states gives the unique opportunity to study interacting atoms in combination of different spin states: high-high (HH), high-low (HL) and low-low (LL).

The magnetic model of two interacting cobalt atoms on one layer of black phosphorus (phosphorene) was constructed within density functional theory by using local density approximation (LDA). Correlations were taken on the level of DFT+U, where Coulomb repulsion parameter makes the similar influence as a bias voltage in